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Coupling Meshfree Peridynamics with Local Finite-Element Models

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ASME 2015 International Mechanical Engineering Congress & Exposition

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CCR Center for Computing Research

U.S. DEPARTMENT OF ENERGY

NNSA National Nuclear Security Administration

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Local-Nonlocal Coupling

VARIABLE LENGTH SCALE IN A PERIDYNAMIC MEDIUM

- Reducing the peridynamic horizon in the vicinity of a local-nonlocal interface improves model compatibility
- Standard peridynamic models do not support a variable horizon
- The peridynamic partial stress formulation does support a variable horizon and can be utilized for local-nonlocal coupling

BLENDING-BASED COUPLING

- Blending-based scheme derived from a single model
- Nonlocal length scale taken to zero in one portion of the domain, recovering local model
- Resulting scheme contains term specific to peridynamics, mitigates ghost forces

OPTIMIZATION-BASED COUPLING

- Model coupling can be cast as an optimization problem
- *Objective function*: Difference between solutions in overlap region
- *Constraints*: Governing equations of the individual models

Collaborators

Marta D'Elia
Mauro Perego
Pavel Bochev

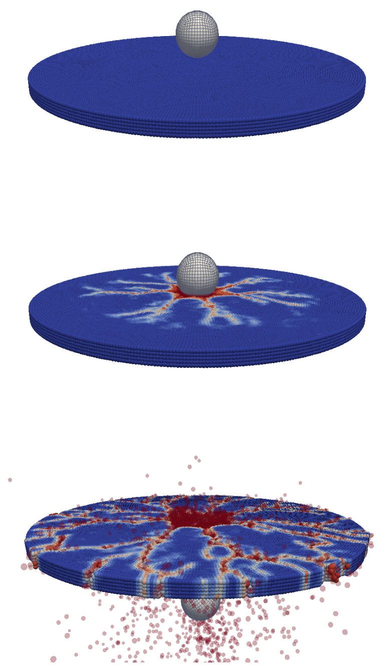
Local-Nonlocal Coupling for Integrated Fracture Modeling

PERIDYNAMICS OFFERS PROMISE FOR MODELING PERVASIVE MATERIAL FAILURE

- Potential to enable rigorous simulation of failure and fracture
- Directly applicable to Sandia's national security mission

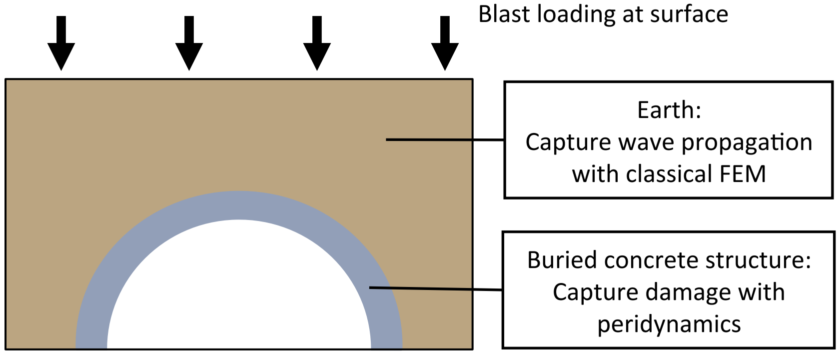
WE SEEK INTEGRATION WITH CLASSICAL FINITE-ELEMENT APPROACHES

- Integration with existing FEM codes provides a delivery mechanism, integration with established analyst workflow
- "Best of both worlds" through combined classical FEM and peridynamic simulations



Simulation of brittle failure

Vision
Apply peridynamics in regions susceptible to material failure



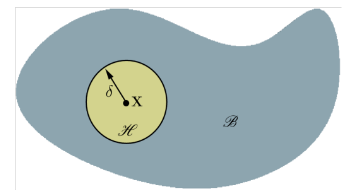
David J. Littlewood, Stewart A. Silling, John A. Mitchell, Pablo D. Seleson, Stephen D. Bond, Michael L. Parks, Daniel Z. Turner, Damon J. Burnett, Jakob Ostien, and Max Gunzburger. Strong Local-Nonlocal Coupling for Integrated Fracture Modeling. Technical report SAND2015-7998. Sandia National Laboratories, Albuquerque, NM and Livermore, CA, 2015.

Peridynamic Theory of Solid Mechanics

Peridynamics is a mathematical theory that unifies the mechanics of continuous media, cracks, and discrete particles

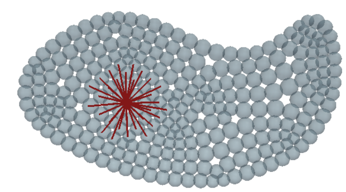
- Peridynamics is a nonlocal extension of continuum mechanics
- Remains valid in presence of discontinuities, including cracks
- Balance of linear momentum is based on an integral equation

$$\rho(\mathbf{x})\ddot{\mathbf{u}}(\mathbf{x},t) = \underbrace{\int_{\mathscr{B}} \left\{ \underline{\mathbf{T}}[\mathbf{x},t]\left\langle \mathbf{x}'-\mathbf{x}\right\rangle - \underline{\mathbf{T}}'[\mathbf{x}',t]\left\langle \mathbf{x}-\mathbf{x}'\right\rangle \right\} \, \mathrm{d}V_{\mathbf{x}'}}_{\text{Divergence of stress replaced with integral of nonlocal forces.}} + \mathbf{b}(\mathbf{x},t)$$



- Peridynamic bonds connect any two material points that interact directly
- Peridynamic forces are determined by force states acting on bonds
- A peridynamic body may be discretized by a finite number of elements

$$\rho(\mathbf{x})\ddot{\mathbf{u}}_h(\mathbf{x},t) = \sum_{i=0}^{N} \left\{ \underline{\mathbf{T}}[\mathbf{x},t]\left\langle \mathbf{x}'_i-\mathbf{x}\right\rangle - \underline{\mathbf{T}}'[\mathbf{x}'_i,t]\left\langle \mathbf{x}-\mathbf{x}'_i\right\rangle \right\} \Delta V_{\mathbf{x}'_i} + \mathbf{b}(\mathbf{x},t)$$



S.A. Silling. Reformulation of elasticity theory for discontinuities and long-range forces. *Journal of the Mechanics and Physics of Solids*, 48:175-209, 2000.

S.A. Silling and E. Askari. A meshfree method based on the peridynamic model of solid mechanics. *Computers and Structures*, 83:1526-1535, 2005.

Silling, S.A. and Lehoucq, R. B. Peridynamic Theory of Solid Mechanics. *Advances in Applied Mechanics* 44:73-168, 2010.

Local-Nonlocal Coupling

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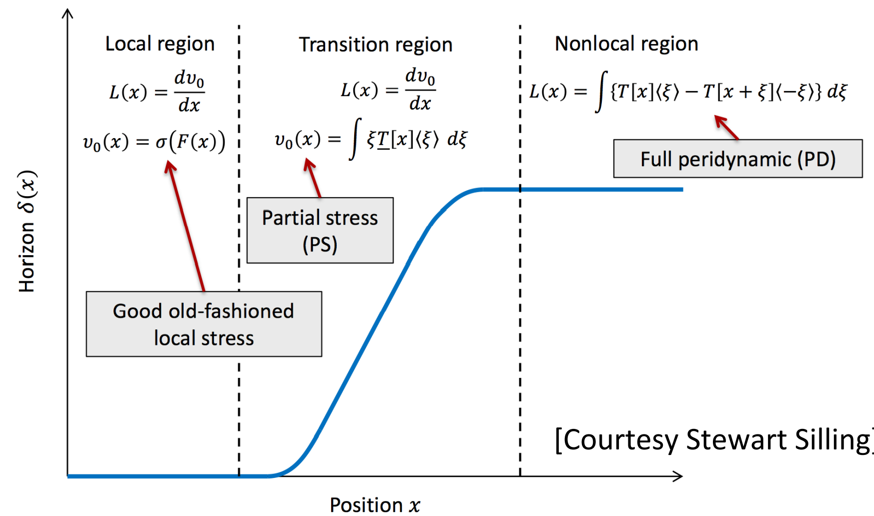
OUTLINE

- Variable length scale in a peridynamic medium
- Blending-based model coupling
- Optimization-based coupling

Variable Nonlocal Length Scale

Reduce peridynamic horizon at local-nonlocal interface to improves model compatibility



[Courtesy Stewart Silling]

STANDARD PERIDYNAMIC MODELS DO NOT SUPPORT A VARIABLE LENGTH SCALE

- Limited support: peridynamic models can support a linearly varying horizon
- *Ghost forces* are proportional to the *second derivative of the horizon*
- Difficulties persist at transition from a constant horizon to a varying horizon

PATH FORWARD

- Seek a formulation that mitigates difficulties associated with a variable horizon
- Potential to greatly reduce model disparity at local-nonlocal interface

Peridynamic Partial Stress Formulation

PERIDYNAMIC STRESS TENSOR

Alternative expression for peridynamic internal force, tis to local theory

$$\mathbf{L}^{\rm pd} = \nabla \cdot \boldsymbol{\nu}^{\rm pd}$$

$$\boldsymbol{\nu}^{\rm pd}(\mathbf{x}) = \frac{1}{2} \int_{\mathcal{S}} \int_0^\infty \int_0^\infty (v+w)^2 \mathbf{f}(\mathbf{x}+v\mathbf{m}, \mathbf{x}-w\mathbf{m}) \otimes \mathbf{m} \, dw \, dv \, d\Omega_{\mathbf{m}}$$

where $$\mathbf{f}(\mathbf{q},\mathbf{p}) = \underline{\mathbf{T}}[\mathbf{p}]\langle \mathbf{q}-\mathbf{p}\rangle - \underline{\mathbf{T}}[\mathbf{q}]\langle \mathbf{p}-\mathbf{q}\rangle$$

PERIDYNAMIC STRESS TENSOR

Under the assumption of a **uniform displacement** field

$$\mathbf{y}(\mathbf{x}+\boldsymbol{\xi}) - \mathbf{y}(\mathbf{x}) = \mathbf{F}\boldsymbol{\xi}$$

The peridynamic stress tensor is greatly simplified

The result is the *peridynamic partial stress*

$$\boldsymbol{\nu}^0 = \int_{\mathcal{H}} \hat{\underline{\mathbf{T}}}(\underline{\mathbf{F}})\langle \boldsymbol{\xi} \rangle \otimes \boldsymbol{\xi} \, dV_{\boldsymbol{\xi}}$$

Lehoucq, R.B., and Silling, S.A. Force flux and the peridynamic stress tensor, *Journal of the Mechanics and Physics of Solids*, 56:1566-1577, 2008.

Silling, S., Littlewood, D., and Seleson, P. Variable horizon in a peridynamic medium. *Accepted for publication*.

Peridynamic Partial Stress Formulation

$$\nu_o(\mathbf{x}) := \int_{\mathcal{H}} \underline{\mathbf{T}}[\mathbf{x}]\langle\xi\rangle \otimes \xi \, dV_{\mathbf{x}'}$$

- GOOD: Supports variable horizon
  - Guaranteed to pass the linear patch test (even with a varying horizon)
  - Provides a natural transition between the full peridynamic formulation and a classical stress-strain formulation (hybrid approach)

- BAD: Is exact only for uniform displacement field
  - Partial stress formulation is not a good candidate for modeling material failure
  - Saving grace: we will apply the partial stress only at local-nonlocal coupling interfaces, which are placed in relatively smooth regions

$$\boldsymbol{\nu}^{\mathrm{pd}} - \boldsymbol{\nu}^{\mathrm{ps}} = O(\delta)O(|\nabla \underline{\mathbf{T}}_1|)$$

S.A. Silling, D.J. Littlewood, and P.D. Seleson. Variable Horizon in a Peridynamic Medium. SAND Report 2014-19088. Sandia National Laboratories, Albuquerque, NM and Livermore, CA, 2014.

Patch Tests for Partial Stress Formulation

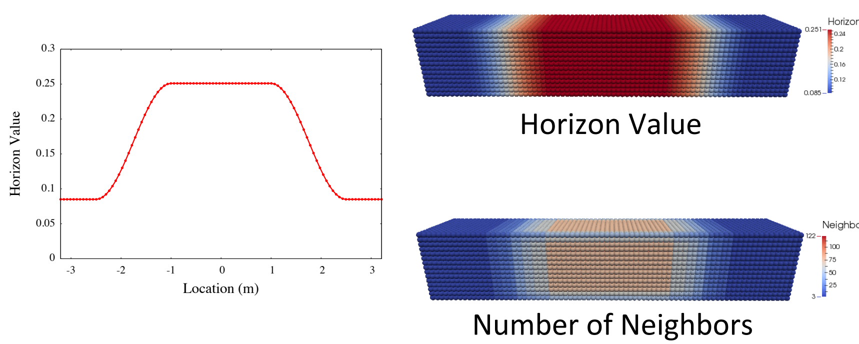
SUBJECT RECTANGULAR BAR TO PRESCRIBED DISPLACEMENT FIELDS

- Examine response under linear and quadratic displacement fields
- Investigate standard formulation with both constant and varying peridynamic horizon
- Investigate partial stress formulation with both constant and varying peridynamic horizon

Elastic Correspondence Material Model

Density	7.8 g/cm^3
Young's Modulus	200.0 GPa
Poisson's Ratio	0.0
Stability Coefficient	0.0

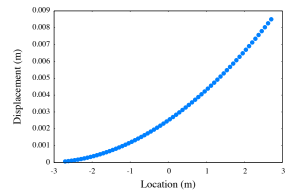
Varying Horizon



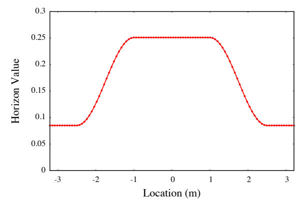
Patch Test: Prescribed Quadratic Displacement

Test set-up

Prescribe quadratic displacement field



Variable horizon

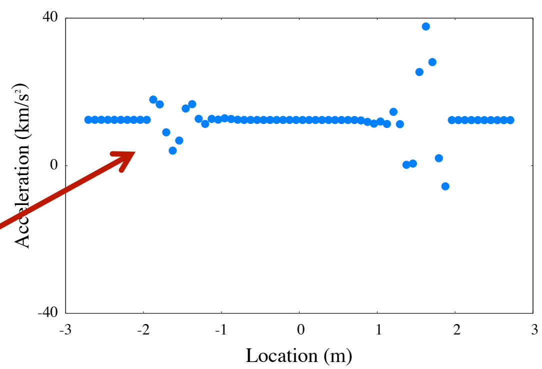


Can the standard model and the partial-stress model recover the expected constant acceleration?

Only the **partial stress** formulation produce the expected result when the horizon is **varying**

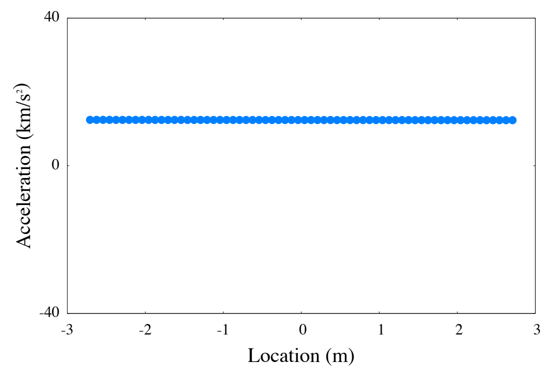
Test Results: Acceleration over the length of the bar

Standard material model



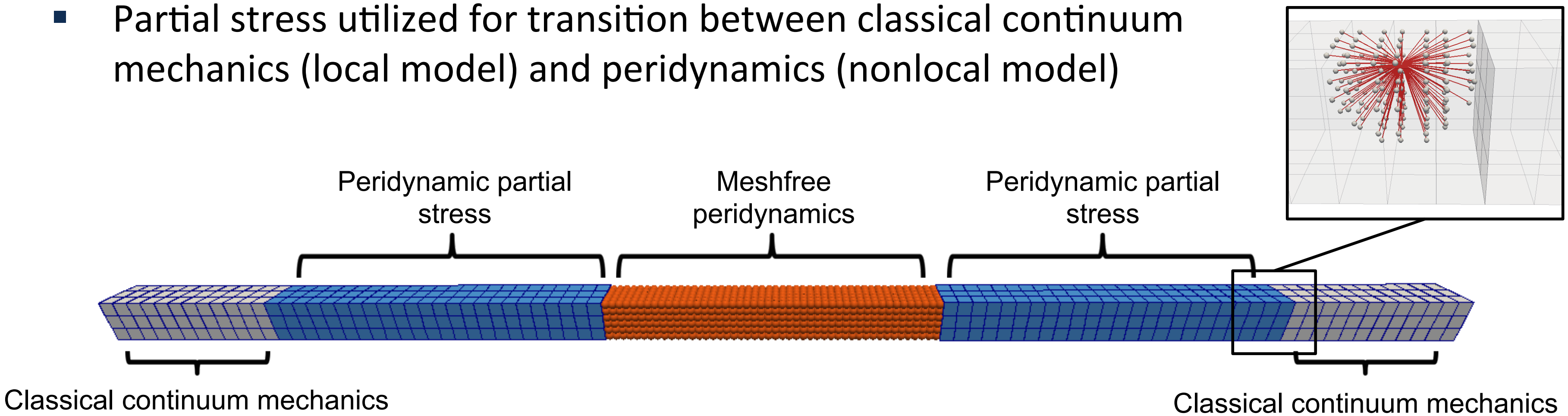
Spurious "ghost forces" present in standard formulation

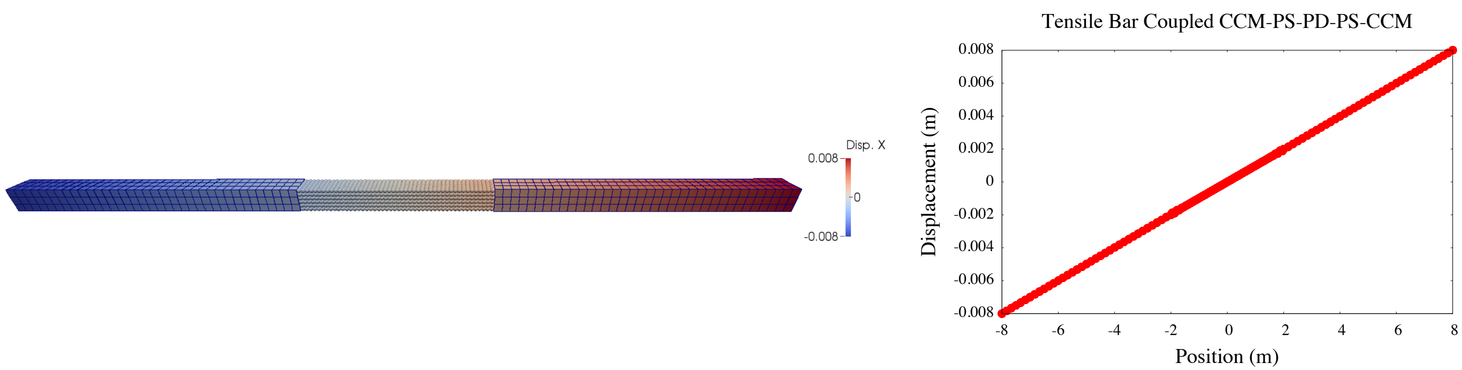
Partial-stress formulation



A Prototype of the Partial Stress Formulation has been Implemented in Coupled *Albany-Peridigm* Code

- Software infrastructure in place for strongly coupled simulations
- Meshfree peridynamic models, peridynamic partial stress, and classical continuum mechanics (FEM) within single executable
- Partial stress utilized for transition between classical continuum mechanics (local model) and peridynamics (nonlocal model)





Local-Nonlocal Coupling

OUTLINE

- Variable length scale in a peridynamic medium
- Blending-based model coupling
- Optimization-based coupling

Blending-Based Approach for Local-Nonlocal Coupling

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APPROACH IS INFORMED BY LINK BETWEEN PERIDYNAMICS AND CLASSICAL LOCAL MODELS

Under the assumption of continuity and smoothness, a peridynamic model reduces to a corresponding local model in the limit of vanishing horizon

Starting point: Bond-based peridynamic equation of motion (start with a single model)

$$\rho(\mathbf{x})\frac{\partial^2\mathbf{u}}{\partial t^2}(\mathbf{x},t) = \int_{\mathcal{B}} \mathbf{f}(\boldsymbol{\eta},\boldsymbol{\xi})\, dV_{\mathbf{x}'} + \mathbf{b}(\mathbf{x},t)$$

Step 1: Introduce *blending function* and split the governing equation into two terms

$$\rho(\mathbf{x})\frac{\partial^2\mathbf{u}}{\partial t^2}(\mathbf{x},t) = \int_{\mathcal{H}(\mathbf{x},\delta)\cap\mathcal{B}} \left(\frac{\beta(\mathbf{x})+\beta(\mathbf{x}')}{2}\right)\mathbf{f}(\boldsymbol{\eta},\boldsymbol{\xi})\, dV_{\mathbf{x}'} + \int_{\mathcal{H}(\mathbf{x},\delta)\cap\mathcal{B}} \left(1-\frac{\beta(\mathbf{x})+\beta(\mathbf{x}')}{2}\right)\mathbf{f}(\boldsymbol{\eta},\boldsymbol{\xi})\, dV_{\mathbf{x}'} + \mathbf{b}(\mathbf{x},t)$$

S.A. Silling and R.B. Lehoucq. Convergence of Peridynamics to Classical Elasticity Theory. *Journal of Elasticity*, 93(1), pp. 13-37, 2008.

P. Seleson, Y.D. Ha, and S. Beneddine. Concurrent coupling of bond-based peridynamics and the navier equation of classical elasticity by blending. *International Journal for Multiscale Computational Engineering,* 13(2), pp. 91-113, 2015.

Blending-Based Approach for Local-Nonlocal Coupling

Step 2: Linearize the right-hand term

$$\rho(\mathbf{x})\frac{\partial^2 \mathbf{u}}{\partial t^2}(\mathbf{x},t) = \int_{\mathcal{H}(\mathbf{x},\delta)\cap\mathcal{B}} \left(\frac{\beta(\mathbf{x})+\beta(\mathbf{x}')}{2}\right) \mathbf{f}(\boldsymbol{\eta},\boldsymbol{\xi})\, dV_{\mathbf{x}'} + \int_{\mathcal{H}(\mathbf{x},\delta)\cap\mathcal{B}} \left(1-\frac{\beta(\mathbf{x})+\beta(\mathbf{x}')}{2}\right) \lambda(\|\boldsymbol{\xi}\|)\,(\boldsymbol{\xi}\otimes\boldsymbol{\xi})\,\boldsymbol{\eta}\, dV_{\mathbf{x}'} + \mathbf{b}(\mathbf{x},t).$$

Step 3: Gradient expansion (Taylor expansion approach)

$$\begin{aligned}\rho(\mathbf{x})\frac{\partial^2 \mathbf{u}}{\partial t^2}(\mathbf{x},t) = & \int_{\mathcal{H}(\mathbf{x},\delta)\cap\mathcal{B}} \left(\frac{\beta(\mathbf{x})+\beta(\mathbf{x}')}{2}\right) \mathbf{f}(\boldsymbol{\eta},\boldsymbol{\xi})\, dV_{\mathbf{x}'} \\ & + \int_{\mathcal{H}(\mathbf{x},\delta)\cap\mathcal{B}} \left(1-\frac{\beta(\mathbf{x})+\beta(\mathbf{x}')}{2}\right) \lambda(\|\boldsymbol{\xi}\|)\,(\boldsymbol{\xi}\otimes\boldsymbol{\xi}) \left[(\boldsymbol{\xi}\cdot\nabla)\,\mathbf{u}(\mathbf{x},t) + \frac{1}{2}\,(\boldsymbol{\xi}\cdot\nabla)\,(\boldsymbol{\xi}\cdot\nabla)\,\mathbf{u}(\mathbf{x},t)\right] dV_{\mathbf{x}'} \\ & + \mathbf{E}(\mathbf{x},t) + \mathbf{b}(\mathbf{x},t).\end{aligned}$$

Step 4: Rearrange and neglect error term

$$\begin{aligned}\rho(\mathbf{x})\frac{\partial^2 \mathbf{u}}{\partial t^2}(\mathbf{x},t) = & \int_{\mathcal{H}(\mathbf{x},\delta)\cap\mathcal{B}} \left(\frac{\beta(\mathbf{x})+\beta(\mathbf{x}')}{2}\right) \mathbf{f}(\boldsymbol{\eta},\boldsymbol{\xi})\, dV_{\mathbf{x}'} \\ & + \left[\int_{\mathcal{H}(\mathbf{x},\delta)\cap\mathcal{B}} \left(1-\frac{\beta(\mathbf{x})+\beta(\mathbf{x}')}{2}\right) \lambda(\|\boldsymbol{\xi}\|)\,\xi_i\xi_j\xi_k dV_{\mathbf{x}'}\right] \frac{\partial u_j}{\partial x_k}(\mathbf{x},t)\,\hat{\mathbf{e}}_i \\ & + \left[\int_{\mathcal{H}(\mathbf{x},\delta)\cap\mathcal{B}} \left(1-\frac{\beta(\mathbf{x})+\beta(\mathbf{x}')}{2}\right) \lambda(\|\boldsymbol{\xi}\|)\,\xi_i\xi_j\xi_k\xi_\ell\, dV_{\mathbf{x}'}\right] \frac{1}{2}\frac{\partial^2 u_j}{\partial x_k x_\ell}(\mathbf{x},t)\,\hat{\mathbf{e}}_i + \mathbf{b}(\mathbf{x},t).\end{aligned}$$

Middle term is unique to local-nonlocal blending approach, eliminates ghost force

S. Badia, M. Parks, P. Bochev, M. Gunzburger, and R. Lehoucq. On atomistic-to-continuum coupling by blending. *Multiscale Modeling and Simulation*, 7:381-406, 2008.

P. Seleson, Y.D. Ha, and S. Beneddine. Concurrent coupling of bond-based peridynamics and the navier equation of classical elasticity by blending. *International Journal for Multiscale Computational Engineering,* 13(2), pp. 91-113, 2015.

Blending-Based Approach for Local-Nonlocal Coupling

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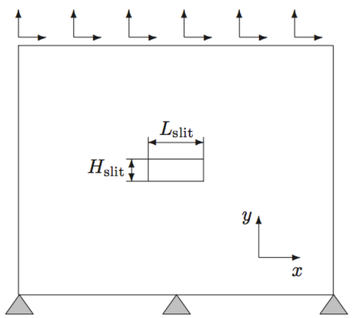
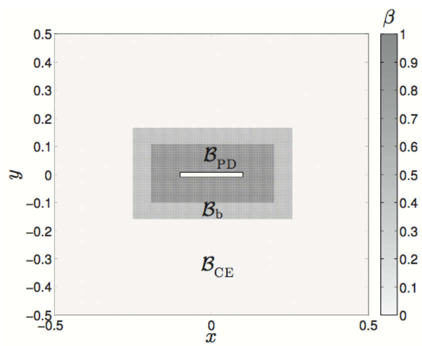
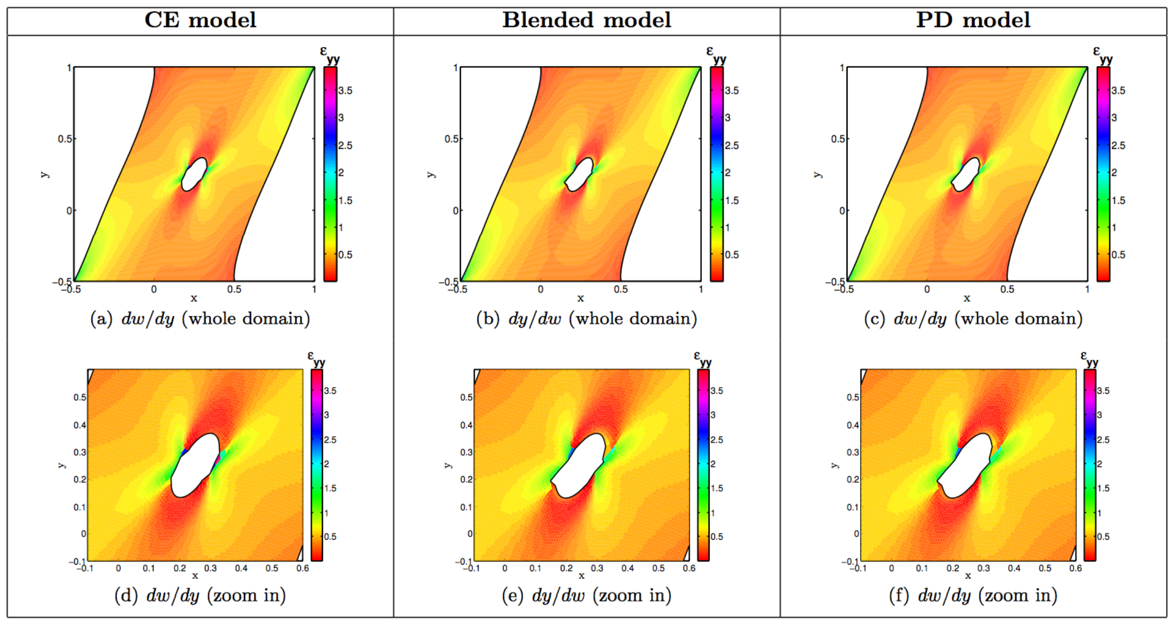
DEMONSTRATION SIMULATION: PLATE WITH CRACK

- Negligible difference between full peridynamic model and coupled model
- Classical local model agrees with peridynamic model far from crack
- Computational time drastically reduced for blended model







P. Seleson, Y.D. Ha, and S. Beneddine. Concurrent coupling of bond-based peridynamics and the navier equation of classical elasticity by blending. *International Journal for Multiscale Computational Engineering,* 13(2), pp. 91-113, 2015.

Local-Nonlocal Coupling

OUTLINE

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Optimization-Based Local-Nonlocal Coupling

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ONGOING EFFORT OF D'ELIA, PEREGO, AND BOCHEV

- Model coupling can be cast as an optimization problem
- *Objective function*: Difference between solutions in overlap region
- *Constraints*: Governing equations of the individual models

APPLICATION OF OPTIMIZATION-BASED COUPLING TO COMPUTATIONAL SOLID MECHANICS

- Appropriate for static and quasi-static problems involving disparate models
- Rigorous mathematical foundation
- Can be applied as a "black box" to couple dissimilar computational domains
- Computational expense is a concern, mitigation strategies being investigated

D'Elia, M., Perego, M., Bochev, P., and Littlewood, D. A coupling strategy for nonlocal and local diffusion models with mixed volume constraints and boundary conditions. *Accepted for publication*.

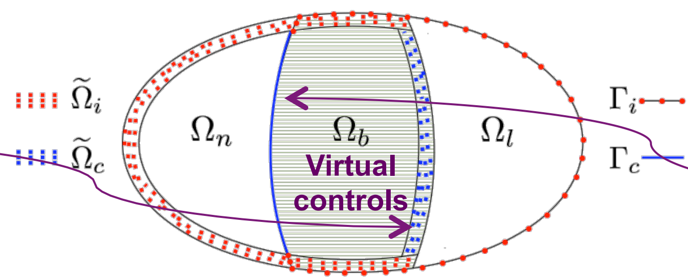
Optimization Based Coupling

Minimize the mismatch between the nonlocal and local models subject to the two models acting independently in Ω_N and Ω_L

$$\min_{u_n, u_l, \theta_n, \theta_l} J(u_n, u_l) = \frac{1}{2}\|u_n - u_l\|^2_{0,\Omega_b} \quad \text{s.t.}$$

Nonlocal

$$\begin{cases} -\mathcal{L}u_n = f_n & \boldsymbol{x} \in \Omega_n \\ u_n = \theta_n & \boldsymbol{x} \in \widetilde{\Omega}_c \\ u_n = 0 & \boldsymbol{x} \in \widetilde{\Omega}_i \end{cases}$$



Local

$$\begin{cases} -\Delta u_l = f_l & \boldsymbol{x} \in \Omega_l \\ u_l = \theta_l & \boldsymbol{x} \in \Gamma_c \\ u_l = 0 & \boldsymbol{x} \in \Gamma_i. \end{cases}$$

Mathematical analysis has established existence, uniqueness of solution to coupled problem

[Courtesy of D'Elia, Perego, and Bochev]

Optimization-Based Coupling: Path Forward

Research & proof-of-principle →  → **Programmatically exercised software**

Utilize agile components approach for development of computational algorithms

- Provide access to adjoints, sensitivites, etc., for adjoint-based fast optimization
- Enable effective transitioning of research ideas into production software

$$\min_{u_n,u_l,\theta_n,\theta_l} J(u_n,u_l) \text{ s.t. } \begin{cases} -\mathcal{L}u_n = f_n & \boldsymbol{x}\in\Omega_n \\ u_n = \theta_n & \boldsymbol{x}\in\widetilde{\Omega}_c \\ u_n = 0 & \boldsymbol{x}\in\widetilde{\Omega}_i \end{cases} \quad \begin{cases} -\Delta u_l = f_l & \boldsymbol{x}\in\Omega_l \\ u_l = \theta_l & \boldsymbol{x}\in\Gamma_c \\ u_l = 0 & \boldsymbol{x}\in\Gamma_i. \end{cases}$$

ROL — Peridigm — Albany

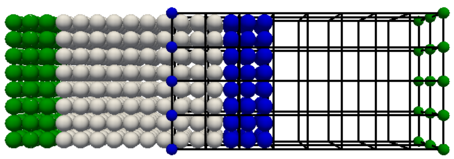
[Courtesy of D'Elia, Perego, and Bochev]

Linear Patch Test Simulation

RECOVERY OF LINEAR SOLUTION USING COUPLED LOCAL-NONLOCAL MODEL

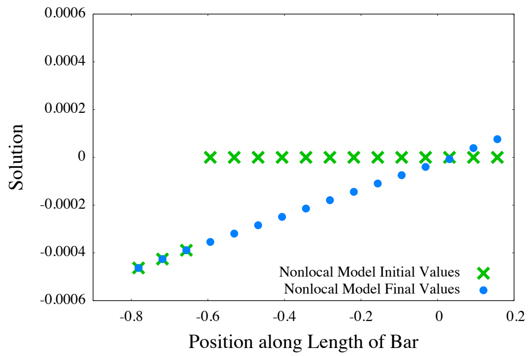
- Boundary conditions applied to ends of bar
  - Linear solution imposed over volumetric region of nonlocal model
  - Standard local boundary conditions applied to local model
- Optimization-based approach successfully couples local and nonlocal models

Problem Set-up

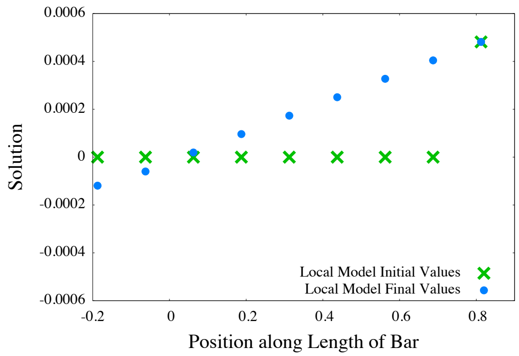


Coupled solution

Solution of local model



Solution of nonlocal model



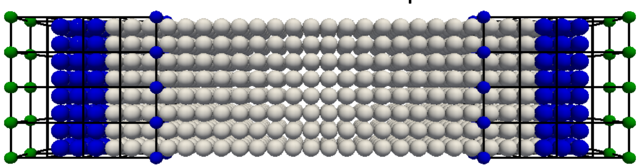
D'Elia, M., Perego, M., Bochev, P., Littlewood, D. A coupling strategy for nonlocal and local diffusion models with mixed volume constraints and boundary conditions. *Accepted for publication.*

Simulation of a Pre-Cracked Bar

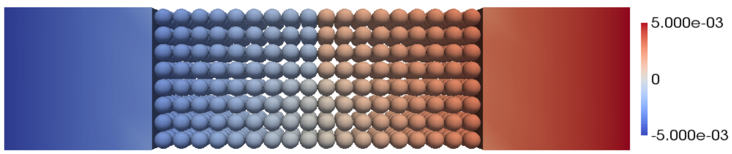
LOCAL BOUNDARY CONDITIONS APPLIED TO PRE-CRACKED BAR

- Boundary conditions applied to local model only
  - Avoids difficulties in applying volume constraints to nonlocal model
- Optimization-based approach successfully couples local and nonlocal models
- Nonlocal model provides solution in vicinity of crack

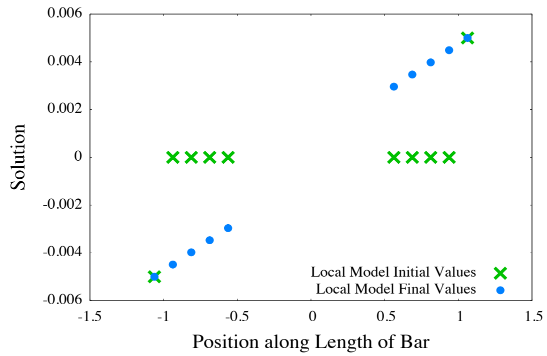
Problem Set-up



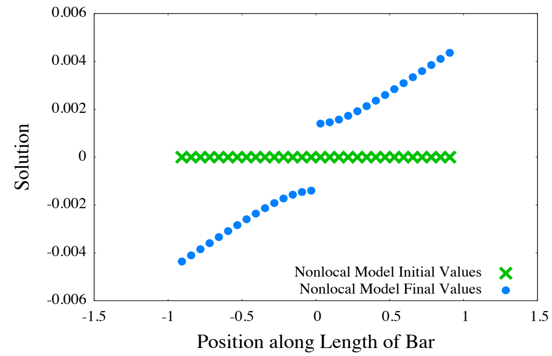
Coupled solution



Solution of local model along top of bar



Solution of nonlocal model along top of bar



D'Elia, M., Perego, M., Bochev, P., Littlewood, D. A coupling strategy for nonlocal and local diffusion models with mixed volume constraints and boundary conditions. *Accepted for publication.*

Questions?

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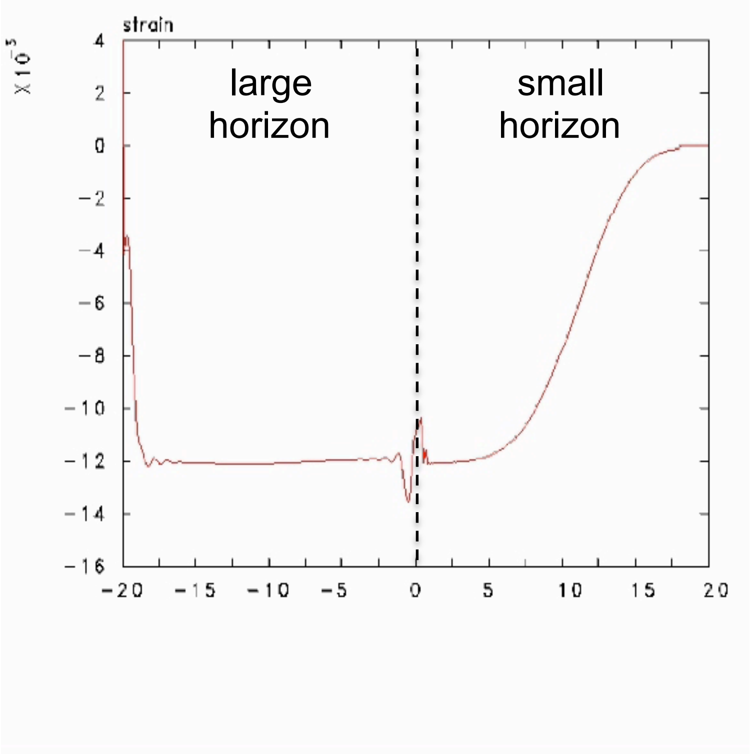
https://peridigm.sandia.gov

Extra Slides

Peridynamic Partial Stress: Wave Propagation through Region of Varying Horizon

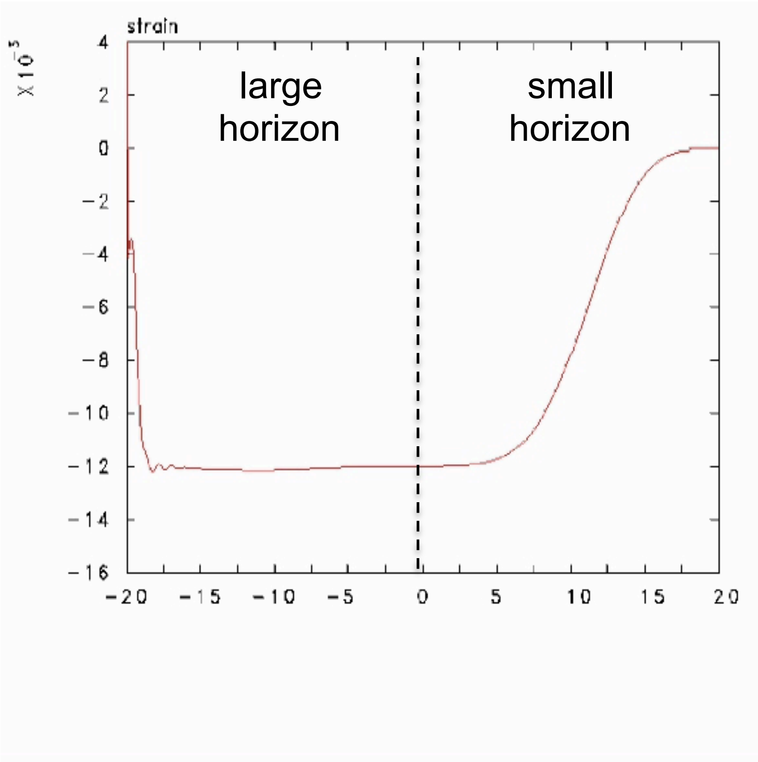
Standard peridynamic model

Numerical artifacts present at transition from large horizon to small horizon



Partial-stress approach

Greatly reduces artifacts, enables smooth transition between large and small horizons



[1] Silling, S., and Seleson, P., Variable Length Scale in a Peridynamic Body, SIAM Conference on Mathematical Aspects of Materials Science, Philadelphia, PA, June 12, 2013.

Peridynamic Partial Stress: What about Performance?

USE OF A VARIABLE HORIZON IMPACTS PERFORMANCE IN SEVERAL WAYS

- Use of a variable horizon can reduce neighborhood size
  - Less computational cost per internal force evaluation
  - Reduces number of unknowns in stiffness matrix for implicit time integration
- Use of a variable horizon can reduce the critical time step
  - Critical time step is strongly dependent on the horizon [1, 2]
  - Smaller time step results in more total steps to solution for explicit transient dynamic simulations
  - Important note: the critical time step for analyses combining peridynamics and classical finite analysis is generally determine by the classical finite elements

Total Number of Bonds
(equal to number of nonzeros in stiffness matrix)

Constant Horizon	92.6 million
Varying Horizon	46.5 million

Stable Time Step [1, 2]
(explicit transient dynamics)

Constant Horizon	2.03e-5 sec.
Varying Horizon	7.15e-6 sec.

[1] S.A. Silling and E. Askari. A meshfree method based on the peridynamic model of solid mechanics. *Computers and Structures*, 83:1526-1535, 2005.

[2] Littlewood, D.J, Thomas, J.D., and Shelton, T.R. Estimation of the Critical Time Step for Peridynamic Models. SIAM Conference on the Mathematical Aspects of Material Science, Philadelphia, Pennsylvania, June 9-12, 2013.